EXCITATION CROSS SECTIONS FOR SOME OF THE STATES OF $2p^4$-3p CONFIGURATION OF NEON AND $4p^4$-5p CONFIGURATION OF KRYPTON

S.H. Koozekanani

The Ohio State University

ElectroScience Laboratory

(formerly Antenna Laboratory)

Department of Electrical Engineering

Columbus, Ohio 43212

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ABSTRACT

Excitation cross sections for some of the $2p^4$-3p upper laser states of neon and $4p^4$-5p states of krypton has been calculated by assuming a fast electron strips away one of the bound valence electrons of the neutral atom in a very short time compared to the relaxation of the ion. Exact wave functions for the upper laser states of neon II and krypton II in terms of pure LS wave functions are found.

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INTRODUCTION

In a previous paper,[1] the method of sudden perturbation was used to calculate the excitation cross section for some of the singly ionized states of Ar II. Experimental measurements of some of the $3p^4$-4p states of argon II has been reported by Bennett.[2]

The method of calculation simply assumes that the Hamiltonian of the atom changes in a very short time compared to the involved relaxation times.[3] To calculate the probability that the atom would be in any one of the many possible states of the perturbed system, one has to expand the eigenfunctions of the unperturbed system in terms of those of the new one. In this problem, we have considered a fast free electron impinging upon a neutral noble gas atom which has six electrons in the outer shell, but after collision, we have instead two free electrons and an atom in an excited ionic state with only five electrons in the valence shells. All this process is supposed to take place in a very short time compared to the relaxation times of the ion. To find the probability $|a_{nj}|^2$ that any excited ionic state is produced, one has to calculate the matrix elements between the initial impinging electron and its final state, matrix elements between one of the bound electron and its final free state and finally matrix elements between the remaining bound electrons of the initial neutral atom and the final ionic excited state. In other words,

$$(1) \qquad |a_{nj}|^2 = \text{const}\ \left| \langle \ell^5, {}^2P_J \,|\, \ell_n^4\, \overline{L}\,\overline{S};\ n\ell',\ LSJM \rangle \right|^2 \left| \left\{ \sum_{\substack{\text{final} \\ \text{states}}} \langle \ell s \,|\, \text{free electron} \rangle \langle \text{initial free elec.} \,|\, \text{final free elec.} \rangle \right\} \right|^2$$

The terms in the braces are proportional to the ionization cross section. $|\ell_n^4\, \overline{L}\,\overline{S},\ n\ell'\ LSJM\rangle$ stands for the excited ionized states and L, S, and J are the total orbital, total spin and the total angular momentum of the system. M is the projection of J over the magnetic z-axis. $\overline{L}$ and $\overline{S}$ are the total spin and orbital angular momenta of the core ℓ^4 electrons. From Eq. (1) and References 1 and 4, we find for the excitation cross section

$$(2) \qquad Q_{\bar{L}\bar{S},LSJ} = [J]\,[j]\,[L]\,[S]\,(\ell^4 \bar{L}\bar{S}\,\{|\,\ell^5 LS)$$

$$\begin{Bmatrix} \bar{L} & \ell & L \\ \bar{S} & s & S \\ \bar{J} & j & J \end{Bmatrix}^2 \int_0^\infty \mathcal{J}_\ell(r)\mathcal{J}_{n\ell}(r)dr \left[\int_0^\infty \mathcal{J}_\ell(r')\,\mathcal{J}_{\ell n}(r')dr\right]^4 Q^+(E)$$

where $\bar{J} = \bar{L} + \bar{S}$, $j = \ell + s$ and the $\mathcal{J}(r)$ are the radial function of the various electrons designated by the subscript. The symbol $[x] = 2x + 1$.

Most of the eigne states, however, cannot be expressed in terms of pure LS or jj coupled states but are rather mixed. To calculate the excitation cross section the exact wave function is needed. One can, however, expand the mixed states ψ_i corresponding to the experimentally found energies E_i in a space spanned by the orthonormal set of LS coupled wave functions. For the configuration of $2p^4$-3p of neon II and $4p^4$-5p of krypton II which are the upper laser states of these ions, exact wave functions have been found.[5] This has been done by letting

$$\psi_i = \sum_j b_{ij}\,|L_iS_iJ_iM_i>$$

and inserting it in the Hamiltonian $H\psi_i = E_i\psi_i$. If both sides of the equation are multiplied by $<L_nS_nJ_nM_n|$ one ends up solving a homogeneous linear set of equations in terms of the expansion coeffieicnts b_{ij}.[6] The Hamiltonian H for the free ion is

$$(3) \qquad H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 - \sum_i \frac{e^2 Z}{r_i} + \sum_{i>j} \frac{e^2}{r_{ij}} + \sum_i \xi_i(r_i)\,\ell_i \cdot s_i$$

where the first two quantities are the usual kinetic energy and the potential terms, while the third is the electrostatic interaction term between the electrons. The last quantity represents the spin orbit interaction. Table I gives the coefficients b_{ij} and the experimental energies E_i to which the wave functions correspond. The calculated energy levels are in close agreement with the experimental values. The discrepancy being less than one per cent.

From Eq. (2) in this paper and Eq. (13) in Reference 1 we can, with the use of coefficients b_{ij}, calculate the excitation cross section for some of the states of $2p^4$-3p configuration of neon and the $4p^4$-5p of krypton. Table II gives these results.

CONCLUSION

Because of the large spin orbit interaction term of KrII in the Hamiltonian of Eq. (3) we notice that the wave functions of krypton II are quite mixed. The state corresponding to the experimental energy of 139103 cm^{-1} although designeated to be a $2p'_{1/2}$ state is approximately 32% $|{}^2P_{1/2}\rangle$, 22% $|{}^4D_{1/2}\rangle$, 22% $|{}^2P_{1/2}\rangle$, 14% $|{}^4P_{1/2}\rangle$ and finally 10% $|{}^2P'_{1/2}\rangle$ state. This shows why excitation to this level, i.e. $\psi_i \equiv E_i(137103\ cm^{-1})$, is not as high as one would have expected it to be. On the other hand neon, more or less seems to be to a great extent, LS coupled.

TABLE I

Expansion Coefficients of the Eigenstates of Hamiltonian of Eq. (3) in terms of LS Coupled Wave Functions. The Underlined are Coefficients of those States to which the Corresponding Experimental Energies are Assigned

		E_{exp} cm^{-1}	^4S	^4P	^4D	^2S	^2P	^2D	$^2P'$	$^2D'$
Neon	$^2S_{1/2}$	c 252800		0.049	0.025	$\underline{0.924}$	0.362		-0.106	
	$^2P_{1/2}$	254294		0.046	0.003	0.378	$\underline{0.895}$		-0.228	
	$^2P_{3/2}$	254167	-0.118	0.053	0.023		$\underline{0.940}$	0.212	-0.230	-0.024
	$^2D_{3/2}$	251524	0.013	-0.007	0.103		0.208	$\underline{0.971}$	-0.043	0.025
	$^4D_{3/2}$	249697	0.012	0.092	$\underline{0.990}$		0.041	0.096	-0.009	0.004
Krypton	$^2S_{1/2}$	142363		0.008	-0.112	$\underline{0.761}$	0.590		0.245	
	$^2P_{1/2}$	139103		0.379	0.470	0.465	$\underline{0.5613}$		-0.321	
	$^2P_{3/2}$	140137	0.037	-0.045	0.624		$\underline{0.674}$	0.323	-0.213	0.072
	$^2D_{3/2}$	141995	0.137	-0.212	0.154		-0.431	$\underline{0.801}$	0.254	0.142
	$^4D_{3/2}$	138381	-0.235	- .334	$\underline{0.704}$		-0.393	-0.421	0.057	0.047

TABLE II

Excitation Cross Sections for NeII and KrII as a Function of Ionization Cross Section: for an Electron Energy $E = 100$ ev $Q^{+}_{Ne}(100\ \text{ev}) = 4.8$ or $6.2 \times 10^{-16}\ \text{cm}^2$ while $Q^{+}_{Kr}(100\ \text{ev}) = 0.87 \times 10^{-16}\ \text{cm}^2$ (Ref. 7)

Neon	$Q(^2S_{1/2}) = 0.027 \times 10^{-2}\ Q^{+}_{Ne}(E)$
	$Q(^2P_{1/2}) = 0.180 \times 10^{-2}\ Q^{+}_{Ne}(E)$
	$Q(^2P_{3/2}) = 0.404 \times 10^{-2}\ Q^{+}_{Ne}(E)$
	$Q(^2D_{3/2}) = 0.021 \times 10^{-2}\ Q^{+}_{Ne}(E)$
	$Q(^4D_{3/2}) = 0.0008 \times 10^{-2}\ Q^{+}_{Ne}(E)$
Krypton	$Q(^2S_{1/2}) = 0.045 \times 10^{-2}\ Q^{+}_{Kr}(E)$
	$Q(^2P_{1/2}) = 0.028 \times 10^{-2}\ Q^{+}_{Kr}(E)$
	$Q(^2P_{3/2}) = 0.144 \times 10^{-2}\ Q^{+}_{Kr}(E)$
	$Q(^2D_{3/2}) = 0.032 \times 10^{-2}\ Q^{+}_{Kr}(E)$
	$Q(^4D_{3/2}) = 0.066 \times 10^{-2}\ Q^{+}_{Kr}(E)$

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